High Pressure – High Temperature Phase Relations in Cobalt and CuS Using the Laser Heated Diamond Anvil Cell

S. Speziale, S-H Shim, T. Duffy (Princeton U.), M. Somayazulu (Arizona State U.)

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Introduction: 3d transition metals are important for understanding planetary cores. A number of high P-T experiments have been reported on Co. We have previously identified a phase transition to a Sm-type structure but also showed that formation of Cobalt oxides could explain at least some of the observed diffraction peaks. On the other hand, Yoo et al reported the transition to a dhcp phase at pressures below 50 GPa and temperatures above 2500 K[1]. We have therefore undertaken a careful evaluation of the effect of different media on the observed high P, T transitions in Co.

CuS is a p-type semiconductor with a complex hexagonal structure characterized by Cu in two different coordinations. X-ray diffraction and vibrational spectroscopy studies document an orthorhombic distortion of the hexagonal lattice at 100 K (ambient pressure). With increasing pressure (at room temperature), the diffraction lines are observed to broaden above 5 GPa followed by complete amorphization above 11 GPa[2-4]. We have undertaken a systematic study of the high P, T behavior of CuS to understand the phase diagram of this material. In the following, we present a progress report on our on-going experiments on Co and CuS.

Methods and Materials: Using the double-sided laser heating system at X17B1, we have studied the high P, T phase diagram in Co and CuS. In the case of Co, we have used Ar as a non-reactive pressure medium (and insulating medium). These in situ measurements would therefore help us explore the effects of the insulating medium and differentiate between chemical reactions and structural transitions at high P,T conditions. In both the sets of experiments, we have collected diffraction data while rotating the sample. This helps eliminate axial temperature gradients while heating and also effects due to sample texturing at high P,T conditions.

Results: In the studies on Co, we have observed no evidence for the reported transition to a dhcp phase. In our studies, the only two stable phases are the hcp or the fcc phases. Our results seem to indicate that the observed transitions in Co where non-inert media such as MgO, NaCl or SiO2 have been used could be a result of the formation of reaction products rather than structural transitions at high pressures and temperatures.

We have observed signatures of two, hitherto unknown transitions in CuS. At room temperature, we have observed a transition to a lower symmetry above 10 GPa in CuS. This new phase is observed to be stable to 20 GPa and temperatures above 2000 K. This lowering of symmetry of the hexagonal phase is in fact consistent with the observed behavior of other sulphides such as PbS and FeS. On further compression, new diffraction lines appear above 25 GPa consistent with our vibrational spectroscopy measurements. This phase is stable up to 35 GPa.

References: [1]C. S. Yoo and H. Cynn, Proc. Of the *IUCr meeting on synchrotron, neutron and Laboratory source crystallography at High Pressures*, Nov. 1998, APS, Chicago; [2]H. Fjellvag et al, Zeit. Krist., **184**, 111 (1988); [3]S. Peiris et al, J. Chem. Phys., **104**, 11 (1996); [4] Y.Takeuchi et al, Zeit. Krist., **173**, 119 (1985).